Stochastic modelling of nonlinear dynamical systems

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Abstract

We develop a general theory dealing with stochastic models for dynamical systems that are governed by various nonlinear, ordinary or partial differential, equations. In particular, we address the problem how flows in the random medium (related to driving velocity fields which are generically bound to obey suitable local conservation laws) can be reconciled with the notion of dispersion due to a Markovian diffusion process.

Contexts

Probabilistic concepts are ubiquitous in diverse areas of nonlinear science. Deterministic dynamical systems may give rise to random transport that is an intrinsic feature of their complex behaviour, augmented by a possible choice of random initial or boundary data and/or suitable scaling limits. Nonequlibrium statistical physics directly employs random processes, Gaussian and non-Gaussian, which ultimately implement a nonlinear transport. Apart from a concrete identification of genuine sources of randomness in the dynamics of classical systems or in quantum theory, quite often we need

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quantitative methods to deal with random-looking phenomena. Basically that refers to situations when origins of randomness are either uncontrollable (allowing merely for probabilistic predictions about the future behaviour of the system) or not definitely settled.

The so-called Schrödinger boundary data and stochastic interpolation problem sets a conceptual and formal basis for a surprisingly rich group of topics. Here, [1], stochastic analysis methods are used to deduce the most likely (generally approximate) underlying dynamics from the given (possibly phenomenological) input-output statistics data, pertaining to a certain dynamical process that is bound to take place in a finite time interval. The pertinent motion scenarios range from processes arising in nonequilibrium phenomena, [2, 3], through classical dynamics of complex systems (deterministic chaos in terms of densities) to searches for a stochastic counterpart of quantum phenomena. They involve random processes that go beyond the standard Gaussian basis and enable a consistent usage of the jump-type processes (Lévy and their perturbed versions) associated with the anomalous transport, [4]. In the diffusion processes context, we have identified the third Newton law for mean velocity fields as being capable to generate anomalous (enhanced) or non-dispersive diffusion-type processes through "perturbations of noise", [3].

Since the stochastic interpretation of various differential equations is our major target, let us mention typical examples that are amenable to our methodology. Those are: Boltzmann, Navier-Stokes, Euler, Burgers (more or less standard transport of matter), Hamilton-Jacobi, Hamilton-Jacobi-Bellmann, Kardar-Parisi-Zhang (an issue of viscosity solutions and the interface profile growth), Fokker-Planck, Kramers (standard random propagation related to the Brownian motion), both linear and nonlinear Schrödinger equations (probabilistic interpretation of solutions, in Euclidean and non-Euclidean versions of the problem, also with reference to an escape over a barrier and decay of a metastable state).

In most of the above cases a natural linearisation of a nonlinear problem is provided by generalized diffusion (heat) equations in their forward and/or backward versions, [1]. On the contrary, a suitable coupled pair of time-adjoint nonlinear diffusion equations admits a linearisation in terms of the familiar Schrödinger equation. That involves Markovian diffusion processes with a feedback (enhancement mechanism named "the Brownian recoil principle"), [3].

Concepts: Schrödinger' s interpolation problem

There are many procedures to deduce an intrinsic dynamics of a physical system from observable data. None of them is free of arbitrary assumptions needed to reduce the level of ambiguity and so none can yield a clean choice of the modelling strategy. As a standard example one may invoke the time series analysis that is a respected tool in the study of complex signals and is routinely utilised for a discrimination between deterministic and random inputs.

Our objective is to reconstruct a *random* dynamics that is consistent with the given input-output statistics data. We shall outline an algorithm allowing to reproduce an admissible microscopic motion scenario under an additional assumption that the sought for dynamics actually *is* a Markovian diffusion process. This reconstruction method is based on solving the so-called Schrödinger boundary-data and interpolation problem.

Given two strictly positive (usually on an open space-interval) boundary probability densities $\rho_0(\vec{x}), \rho_T(\vec{x})$ for a process with the time of duration $T \geq 0$. One can single out a unique Markovian diffusion process which is specified by solving the Schrödinger boundary data problem:

$$m_T(A, B) = \int_A d^3x \int_B d^3y \, m_T(\vec{x}, \vec{y}) \tag{1}$$

$$\int d^3y \, m_T(\vec{x}, \vec{y}) = \rho_0(\vec{x}) \, , \int d^3x \, m_T(\vec{x}, \vec{y}) = \rho_T(y) \tag{2}$$

where the joint probability distribution has a density

$$m_T(\vec{x}, \vec{y}) = u_0(\vec{x}) \, k(\vec{x}, 0, \vec{y}, T) \, v_T(\vec{y}) \tag{3}$$

and the two unknown functions $u_0(\vec{x})$, $v_T(\vec{y})$ come out as (unique) solutions, of *the same sign,* of the integral identities. To this end, we need to have at our disposal a continuous bounded strictly positive (ways to relax this assumption are known) function $k(\vec{x}, s, \vec{y}, t), 0 \leq s < t \leq T$, which for our purposes (an obvious way to secure the Markov property) is chosen to be represented by familiar Feynman-Kac integral kernels of contractive dynamical semigroup operators:

$$k(\vec{y}, s, \vec{x}, t) = \int exp[-\int_s^t c(\vec{\omega}(\tau), \tau) d\tau] d\mu_{(\vec{x},t)}^{(\vec{y},s)}(\omega) \tag{4}$$

In the above, $d\mu^{(\vec{y},s)}_{(\vec{x},t)}(\omega)$ is the conditional Wiener measure over sample paths of the standard Brownian motion. (Another choice of the measure allows to extend the framework to jump-type processes.)

The pertinent (interpolating) Markovian process can be ultimately determined by means of positive solutions (it is desirable to have them bounded) of the adjoint pair of generalised heat equations:

$$\partial_t u(\vec{x},t) = \nu \triangle u(\vec{x},t) - c(\vec{x},t)u(\vec{x},t) \tag{5}$$

$$\partial_t v(\vec{x},t) = -\nu \triangle v(\vec{x},t) + c(\vec{x},t)v(\vec{x},t) \ . \tag{6}$$

Here, a function $c(\vec{x},t)$ is restricted only by the positivity and continuity demand for the kernel.

Solutions, upon suitable normalisation give rise to the Markovian diffusion process with the *factorised* probability density $\rho(\vec{x},t) = u(\vec{x},t)v(\vec{x},t)$ which, while evolving in time, interpolates between the boundary density data $\rho(\vec{x},0)$ and $\rho(\vec{x},T)$. The interpolation admits an Itô realisation with the respective forward and backward drifts defined as follows:

$$\vec{b}(\vec{x},t) = 2\nu \frac{\nabla v(\vec{x},t)}{v(\vec{x},t)} \tag{7}$$

$$\vec{b}_*(\vec{x},t) = -2\nu \frac{\nabla u(\vec{x},t)}{u(\vec{x},t)} \tag{8}$$

in the prescribed time interval $[0,T]$.
For the forward interpolation, the familiar Fokker-Planck (second Kolmogorov) equation holds true:

$$\partial_t \rho(\vec{x},t) = \nu \triangle \rho(\vec{x},t) - \nabla[\vec{b}(\vec{x},t)\rho(\vec{x},t)] \tag{9}$$

with $\rho(\vec{x},0)$ given, while for the backward interpolation (starting from $\rho(\vec{x},T)$) we have:

$$\partial_t \rho(\vec{x},t) = -\nu \triangle \rho(\vec{x},t) - \nabla[\vec{b}_*(\vec{x},t)\rho(\vec{x},t)] \ . \tag{10}$$

The drifts are gradient fields, $curl\, \vec{b} = 0$. As a consequence, those that are allowed by any prescribed choice of the function $c(\vec{x},t)$ *must* fulfill the compatibility condition

$$c(\vec{x},t) = \partial_t \Phi \ + \ \frac{1}{2}(\frac{b^2}{2\nu} + \nabla b) \tag{11}$$

which establishes the Girsanov-type connection of the forward drift $\vec{b}(\vec{x},t) = 2\nu\nabla\Phi(\vec{x},t)$ with the Feynman-Kac potential $c(\vec{x},t)$. In the considered Schrödinger's interpolation framework, the forward and backward drift fields are connected by the identity $\vec{b}_* = \vec{b} - 2\nu\nabla ln\rho$.

For Markovian diffusion processes the notion of the *backward* transition probability density $p_*(\vec{y},s,\vec{x},t)$ can be consistently introduced on each finite time interval, say $0 \leq s < t \leq T$:

$$\rho(\vec{x},t)p_*(\vec{y},s,\vec{x},t) = p(\vec{y},s,\vec{x},t)\rho(\vec{y},s) \tag{12}$$

so that $\int \rho(\vec{y},s)p(\vec{y},s,\vec{x},t)d^3y = \rho(\vec{x},t)$ and $\rho(\vec{y},s) = \int p_*(\vec{y},s,\vec{x},t)\rho(\vec{x},t)d^3x$.

The transport (density evolution) equations refer to processes running in opposite directions in a fixed, common for both time-duration period. The forward one executes an interpolation from the Borel set A to B, while the backward one executes an interpolation from B to A.

Let us mention at this point that various partial differential equations associated with Markovian diffusion processes are known *not* to be invariant under time reversal. That implies dissipation and links them with irreversible physical phenomena. However, the correspoding processes are known to admit a *statistical inversion* and asking for a statistical past of the process makes sense.

In particular, the knowledge of the Feynman-Kac kernel implies that the transition probability density of the forward process reads:

$$p(\vec{y},s,\vec{x},t) = k(\vec{y},s,\vec{x},t)\frac{v(\vec{x},t)}{v(\vec{y},s)} \ . \tag{13}$$

while the corresponding transition probability density of the backward process has the form:

$$p_*(\vec{y},s,\vec{x},t) = k(\vec{y},s,\vec{x},t)\frac{u(\vec{y},s)}{u(\vec{x},t)} \ . \tag{14}$$

Obviously in the time interval $0 \leq s < t \leq T$ there holds:

$$u(\vec{x},t) = \int u_0(\vec{y})k(\vec{y},s,\vec{x},t)d^3y \tag{15}$$

$$v(\vec{y},s) = \int k(\vec{y},s,\vec{x},T)v_T(\vec{x})d^3x \ . \tag{16}$$

Consequently, we have fully determined the underlying (Markovian) random motions, forward and backward, respectively. All that accounts for perturbations of (and conditioning upon) the Wiener noise.

Particularities

If we consider a fluid in thermal equilibrium as the noise carrier, a kinetic theory viewpoint amounts to visualizing the constituent molecules that collide not only with each other but also with the tagged (colloidal) particle, so *enforcing* and *maintaining* its observed erratic motion. The Smoluchowski approximation takes us away from those kinetic theory intuitions by projecting the phase-space theory of random motions into its configuration space image which is a spatial Markovian diffusion process, whose formal infinitesimal encoding reads:

$$d\vec{X}(t) = \frac{\vec{F}}{m\beta}dt + \sqrt{2D}d\vec{W}(t) \ . \tag{17}$$

In the above m stands for the mass of a diffusing particle, β is a friction parameter, D is a diffusion constant and $\vec{W}(t)$ is a normalised Wiener process. The Smoluchowski forward drift can be traced back to a presumed selective action of the external force $\vec{F} = -\vec{\nabla}V$ on the Brownian particle that has a negligible effect on the thermal bath but in view of frictional resistance imparts to a particle the *mean* velocity $\vec{F}/m\beta$ on the β^{-1} time scale.

The noise carrier (fluid in the present considerations) statistically remains in the state of rest, with *no* intrinsic mean flows, hence unperturbed in the mean (all other cases we associate with the term "perturbations of noise"). At the first glance, a formal replacement of the Smoluchowski forward drift in Eq. (17) by any space-time dependent driving velocity field would suggest a legitimate procedure to implement a net transport that would combine dispersion due to a diffusion process with deterministic mean flows due to external agencies (consider Euler, Navier-Stokes or Burgers velocity fields as reference examples). However the situation is not that simple.

It is well known that a spatial diffusion (Smoluchowski) approximation of the phase-space process, allows to reduce the number of *independent* local

conservation laws to two only. Therefore the Fokker-Planck equation can always be supplemented by another (independent) partial differential equation to form a *closed* system. If we assign a probability density $\rho_0(\vec{x})$ with which the initial data $\vec{x}_0 = \vec{X}(0)$ are distributed, then the emergent Fick law would reveal a statistical tendency of particles to flow away from higher probability residence areas. This feature is encoded in the corresponding Fokker-Planck equation: $\partial_t \rho = -\vec{\nabla} \cdot (\vec{v}\rho) = -\vec{\nabla} \cdot [(\frac{\vec{F}}{m\beta} - D\frac{\vec{\nabla}\rho}{\rho})\rho]$ where a diffusion current velocity is $\vec{v}(\vec{x},t) = \vec{b}(\vec{x},t) - D\frac{\vec{\nabla}\rho(\vec{x},t)}{\rho(\vec{x},t)}$ while the forward drift reads $\vec{b}(\vec{x},t) = \frac{\vec{F}}{m\beta}$. Clearly, the local diffusion current (a local flow that might be experimentally observed for a cloud of suspended particles in a liquid) $\vec{j} = \vec{v}\rho$ gives rise to a non-negligible matter transport on the ensemble average, even if no intrinsic mean flows are in existence in the random medium.

We may surely consider a formal replacement of the previous $\frac{\vec{F}}{m\beta}$ by a local velocity field $\vec{v}(\vec{x},t)$. However, irrespectively of whether we utilize $\frac{\vec{F}}{m\beta}$ or $\vec{v}(\vec{x},t)$ in the formalism, the velocity field *must* obey the natural (local) momentum conservation law which directly originates from the rules of the Itô calculus for Markovian diffusion processes and from the first moment equation in the diffusion approximation (!) of the Kramers theory:

$$\partial_t \vec{v} + (\vec{v} \cdot \vec{\nabla})\vec{v} = \vec{\nabla}(\Omega - Q) \ . \tag{18}$$

An effective potential function $\Omega(\vec{x})$ can be expressed in terms of the Smoluchowski forward drift $\vec{b}(\vec{x}) = \frac{\vec{F}(\vec{x})}{m\beta}$ as follows: $\Omega = \frac{\vec{F}^2}{2m^2\beta^2} + \frac{D}{m\beta}\vec{\nabla} \cdot \vec{F}$. That is to be compared with Eq. (11) which governs the more general space-time dependent situation.

Moreover, in the would-be Euler equation (18), instead of the standard pressure term, there appears a contribution from a probability density ρ-dependent potential $Q(\vec{x},t)$. It is given in terms of the so-called osmotic velocity field $\vec{u}(\vec{x},t) = D\vec{\nabla}\, ln\rho(\vec{x},t)$: $Q(\vec{x},t) = \frac{1}{2}\vec{u}^2 + D\vec{\nabla} \cdot \vec{u}$ and is generic to a local momentum conservation law respected by isothermal Markovian diffusion processes.

To analyze general perturbations of the medium and then the resulting intrinsic (mean) flows, a function $\vec{b}(\vec{X}(t),t)$, must replace the Smoluchowski drift. Under suitable restrictions, we can relate probability measures corresponding to different (in terms of forward drifts !) Fokker-Planck equations

and processes by means of the Cameron-Martin-Girsanov theory of measure transformations, [1]. For suitable forward drifts which are gradient fields that yields the most general form of an auxiliary potential (cf. Eq. (11)) $\Omega(\vec{x},t) = 2D[\partial_t\phi + \frac{1}{2}(\frac{\vec{b}^2}{2D} + \vec{\nabla}\cdot\vec{b})]$. We denote $\vec{b}(\vec{x},t) = 2D\vec{\nabla}\phi(\vec{x},t)$.

Mathematical features of the formalism appear to depend crucially on the properties (like continuity, local and global boundedness, Rellich class) of the auxiliary potential Ω. Let us consider a bounded from below (local boundedness from above is useful as well), continuous function $\Omega(\vec{x},t)$. Then, by means of the gradient field ansatz for the diffusion current velocity ($\vec{v} = \vec{\nabla}S \rightarrow \partial_t\rho = -\vec{\nabla}\cdot[(\vec{\nabla}S)\rho]$) we can transform the local momentum conservation law of a Markovian diffusion process to a universal Hamilton-Jacobi form:

$$\Omega = \partial_t S + \frac{1}{2}|\vec{\nabla}S|^2 + Q \tag{19}$$

where $Q(\vec{x},t)$ was defined before. By applying the gradient operation we recover the conservation law (18).

In the above, the contribution due to Q is a direct consequence of an initial probability measure choice for the diffusion process, while Ω does account for an appropriate forward drift of the process via Eq. (19).

Thus, in the context of Markovian diffusion processes, we can consider a *closed* system of partial differential equations which comprises the continuity equation $\partial_t\rho = -\vec{\nabla}(\vec{v}\rho)$ and the Hamilton-Jacobi equation, plus suitable initial (and/or boundary) data. The underlying isothermal diffusion process is specified uniquely. Those two partial differential equations set ultimate limitations in the old-fashioned problem of "how much nonlinear" and "how much space-time dependent" the driving velocity field can be to yield a consistent stochastic diffusion process (or the Langevin-type dynamics)

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